

# Coulomb energy difference as a probe of isospin-symmetry breaking in the upper $fp$ -shell nuclei

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(Dated: July 27, 2012)

The anomaly in Coulomb energy differences (CED) between the isospin  $T = 1$  states in the odd-odd  $N = Z$  nucleus  $^{70}\text{Br}$  and the analogue states in its even-even partner  $^{70}\text{Se}$  has remained a puzzle. This is a direct manifestation of isospin-symmetry breaking in effective nuclear interactions. Here, we perform large-scale shell-model calculations for nuclei with  $A = 66 - 78$  using the new filter diagonalization method based on the Sakurai-Sugiura algorithm. The calculations reproduce well the experimental CED. The observed negative CED for  $A = 70$  are accounted for by the cross-shell neutron excitations from the  $fp$ -shell to the  $g_{9/2}$  intruder orbit with the enhanced electromagnetic spin-orbit contribution at this special nucleon number.

PACS numbers: 21.10.Sf, 21.30.Fe, 21.60.Cs, 27.50.+e

Isospin is a fundamental concept in nuclear and particle physics. The isospin symmetry was introduced under the assumption of charge independence of the nuclear force [1]. Historically, the study of this symmetry led directly to the discovery and understanding of quarks. However, it is well known that this symmetry is only approximate because of the existence of the Coulomb interaction and isospin-breaking interactions among nucleons, leading to small differences, for example, in the binding energy of mirror-pair nuclei and in the excitation energy of the same spin,  $J$ , between isobaric analogue states (IAS) of the same isospin,  $T$ .

A nucleus is a quantum many-body system with finite size, which generally shows two unique features in structure: the shell effect with the presence of strong spin-orbit interaction [2] and the nuclear deformation associated with collective motion [3]. To properly describe these aspects in the framework of nuclear shell models, effective interactions must be involved. Thus the effects of isospin-symmetry breaking can manifest themselves through structure changes in the vicinity of the  $N = Z$  line, providing information on the  $T_z$ -dependence of the effective interactions. The effects have been extensively studied for nuclei in the upper  $sd$ - and the lower  $fp$ -shell regions (see Ref. [4] for review), where a remarkable agreement between experimental mirror energy differences (MED) and shell-model calculations has been found, allowing a clear identification of the origin of isospin-symmetry breaking in effective nuclear interactions.

The Coulomb energy difference (CED), defined by

$$\text{CED}(J) = E_x(J, T = 1, T_z = 0) - E_x(J, T = 1, T_z = 1), \quad (1)$$

is often regarded as a measure of isospin-symmetry breaking in effective nuclear interactions which include the Coulomb force [5, 6]. In Eq. (1),  $E_x(J, T, T_z)$  are the excitation energies of IAS with spin  $J$  and isospin  $T$ , distinguished by different  $T_z$  (the projection of  $T$ ).

More complex shell structures are expected for heavier mass regions. In the upper  $fp$ -shell, for example, abrupt struc-

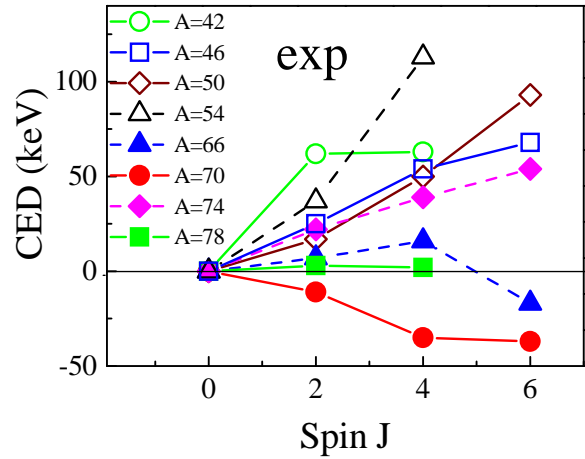


FIG. 1: (Color online) Experimental CED between the isospin  $T = 1$  states in odd-odd  $N = Z$  nuclei and the IAS in even-even nuclei for mass numbers  $A = 42 - 78$ . Data were taken from Refs. [4–6, 11].

ture changes along the  $N = Z$  line [7] and the phenomenon of shape coexistence [8–10] are known. Being pushed down to the lower shell by the spin-orbit interaction [2], the  $g_{9/2}$  intruder orbit and its interplay with the  $fp$ -shell orbits play a key role in the overall structure. However, the influence of these structure changes on CED has not been explored. In Fig. 1, we show the experimental CED for nuclei with mass numbers  $A = 42$  to  $78$ , together with the very recent data of the  $4_1^+$  and  $6_1^+$  states in  $A = 66$  [11]. One observes that, while most of the CED values are positive, only the mass number  $A = 70$  has negative CED [6, 12]. There have been suggestions to explain such an anomalous behavior but without much success. In Ref. [6], it was suggested that this behavior could be attributed to the Thomas-Ehrman effect [13, 14] of the loosely bound proton in  $^{70}\text{Br}$ . However, as pointed out in Ref. [5], this suggestion cannot explain the observed positive CED in other systems such as  $A = 66, 74, 78$  because these systems

have similar binding energy differences as in  $A = 70$ . In Ref. [5], it was suggested that the anomaly may be qualitatively accounted for by small variations in the Coulomb energy due to shape differences in the pair of nuclei. The authors in Ref. [5] tried to argue that such deformation changes occur only for a prolate shape, and not for transition from an oblate ground state to excited configurations [5]. However, recent measurements and theoretical calculations indicate that both  $^{70}\text{Br}$  and  $^{70}\text{Se}$  are associated with an oblate shape [12, 15]. Most recently, the anomalous behavior has been suggested as due to different mixing of competing shapes within the members of the isobaric multiplet [11].

In the past few years, experimental data for mirror nuclei above the doubly magic  $^{56}\text{Ni}$  have become available. The MED in the  $A \sim 60$  mass region were discussed [16, 17]. It was reported that the contribution to MED from the electromagnetic spin-orbit term  $\epsilon_{ls}$  is significant, while the monopole Coulomb term  $\epsilon_{ll}$  is not. Here, detailed variations in nuclear shell structure enter into the discussion. Energy shifts due to the  $\epsilon_{ls}$  term increase the gap between the  $p_{3/2}$ ,  $f_{5/2}$  and the  $g_{9/2}$  orbit for neutrons but reduce that for protons. As a consequence, excitations involving these orbits contribute differently to MED. We have recently investigated MED between the isobaric analogue states in the mirror-pair nuclei  $^{67}\text{Se}$  and  $^{67}\text{As}$  using large-scale shell-model calculations [18]. The calculations reproduced well the experimental MED [19], and suggested that the  $\epsilon_{ls}$  term provides the main contribution to the observed MED values. The negative MED values observed in the  $A = 67$  mirror nuclei were explained by the single-particle-energy shifts due to the  $\epsilon_{ls}$  contribution. We may thus expect that the  $\epsilon_{ls}$  term plays a similarly important role for the anomaly in CED in the  $A = 70$  IAS.

To study CED and probe isospin-symmetry breaking in finite nuclei, calculations for energy levels with an accuracy of a few keV are required. The current state-of-the-art shell-model calculations with the m-scheme using the Lanczos diagonalization method [20] can handle a matrix dimension of the order of  $10^{10}$ . However, it is difficult for the Lanczos method to obtain solutions for  $T \sim 1$  states in odd-odd  $N = Z$  nuclei under the isospin-symmetry breaking with the Coulomb interaction. As for instance, it is impossible to obtain the  $T \sim 1$ ,  $J = 4$  state because of the presence of numerous  $T \sim 0$  states below it. To solve this problem, a breakthrough in shell-model calculations is needed. Quite recently, the filter diagonalization method for large-scale shell-model calculations has been proposed by some of us [21], which is based on a new algorithm for diagonalization suggested by Sakurai and Sugiura [22] (called the SS method). The filter diagonalization procedure can overcome the difficulty mentioned above [23].

In this Letter, shell-model calculations are performed by using the filter diagonalization method in the  $pf_{5/2}g_{9/2}$  model space. We employ the recently-proposed JUN45 interaction [24], a realistic effective interaction based on the Bonn-C potential and adjusted to the experimental data of the  $A = 63 \sim 96$  mass region. We try to solve a general shell-model eigen-

value equation

$$\hat{H}|\Phi_k\rangle = e_k|\Phi_k\rangle, \quad (2)$$

where  $\hat{H}$  is the shell-model Hamiltonian, and  $e_k$  and  $|\Phi_k\rangle$  are eigenvalues and eigenfunctions, respectively. The spirit of the filter diagonalization method [21] is that in order to reduce the large-scale eigenvalue problem to a smaller one, one introduces moments  $\mu_p$  ( $p = 0, 1, 2, \dots$ ) defined by the Cauchy's integral

$$\mu_p = \frac{1}{2\pi i} \int_{\Gamma} \langle \psi | \frac{(z - \epsilon)^p}{z - \hat{H}} | \phi \rangle dz, \quad (3)$$

where  $|\psi\rangle$  and  $|\phi\rangle$  are arbitrary wave functions,  $\epsilon$  is a given energy for a target region, and  $\Gamma$  is an integration contour. Following the SS method [22], one can extract the eigenvalues  $e_k$  ( $k \in \Gamma$ ) inside the closed curve  $\Gamma$  from these moments. In this way, the large-scale eigenvalue problem inside  $\Gamma$  is reduced to

$$Mx = \lambda Nx, \quad (4)$$

where  $M$  and  $N$  are  $n \times n$  Hankel matrices expressed by the moments  $\mu_p$  and the eigenvalues  $\lambda_0, \dots, \lambda_{n-1}$  in the interior of  $\Gamma$ . After diagonalizing (4), one obtains the eigenvalues  $e_k = \epsilon + \lambda_k$  inside the integration contour  $\Gamma$  (Details were discussed in Ref. [21]). For the present case, we apply filter diagonalizations by taking the  $T_-|\psi_f^{T=1}\rangle$  state as  $|\psi\rangle$  and  $|\phi\rangle$  in Eq. (3) for the odd-odd  $N = Z$  nucleus, where  $T_-$  is the lowering operator of isospin and  $|\psi_f^{T=1}\rangle$  is an isovector  $T = 1$  state with spin  $J$  in the even-even  $N = Z + 2$  nucleus. Therefore  $T_-|\psi_f^{T=1}\rangle$  is a good approximation to the wave function of the CED state. In sharp contrast to the usual Lanczos method, by taking  $\Gamma$  around the energy of this state, the filter diagonalization handles only the target CED state. This is the reason why the filter diagonalization can succeed in the calculation.

CED have been studied in the shell-model framework by using the formalism introduced by Zuker *et al.* [25]. In this description, the Coulomb interaction is separated into a monopole term  $V_{Cm}$  and a multipole term  $V_{CM}$ . While  $V_{Cm}$  accounts for single-particle and bulk effects,  $V_{CM}$  contains all the rest. The monopole term  $V_{Cm}$  is further divided into the single-particle correction  $\epsilon_{ll}$ , the radial term  $V_{Cr}$ , and the electromagnetic spin-orbit term  $\epsilon_{ls}$ . It has been reported that the radial term  $V_{Cr}$  does not give a correct description in the lower part of the upper  $fp$ -shell [16], and furthermore, this term may be important only for high-spin states [18]. Therefore,  $V_{Cr}$  is not considered in the present calculation. The isospin nonconserving interaction is also neglected for the upper half of the  $fp$ -shell region because the  $f_{7/2}$  orbit is almost not active.

The single-particle energy shift  $\epsilon_{ls}$  takes into account the relativistic spin-orbit interaction [26]. This interaction originates from the Larmor precession of nucleons in electric fields due to their magnetic moments, which, as well known, affects the single-particle energy spectrum.  $\epsilon_{ls}$  can be written as [26]

$$\epsilon_{ls} = (g_s - g_l) \frac{1}{2m_N^2 c^2} \left( \frac{1}{r} \frac{dV_c}{dr} \right) \langle \hat{l} \cdot \hat{s} \rangle, \quad (5)$$

where  $m_N$  is the nucleon mass and  $V_c$  is the Coulomb potential due to the  $^{56}\text{Ni}$  core. The free values of the gyromagnetic factors,  $g_s^\pi = 5.586$ ,  $g_l^\pi = 1$  for protons and  $g_s^v = -3.828$ ,  $g_l^v = 0$  for neutrons, are used. By assuming a uniformly charged sphere,  $\epsilon_{ls}$  is calculated in the present work by using the harmonic-oscillator single-particle wave functions. Depending on proton or neutron orbits, the shift can have opposite signs. It depends also on the spin-orbit coupling, as for instance  $\langle \hat{l} \cdot \hat{s} \rangle = l/2$  when  $j = l + s$  and  $\langle \hat{l} \cdot \hat{s} \rangle = -(l + 1)/2$  when  $j = l - s$ . As one will see, these strongly affect the results in the following discussion.

With inclusion of the  $V_{CM}$ ,  $\epsilon_{ll}$ , and  $\epsilon_{ls}$  terms, shell-model calculations using the filter diagonalization method are carried out in the  $pf_{5/2}g_{9/2}$  model space for odd-odd  $N = Z$  nuclei and their even-even IAS partners for  $A = 66, 70, 74$ , and  $78$ . In Fig. 2, the calculated CED are compared with available experimental data. As can be seen, the calculation reproduces the experimental CED remarkably well. In particular, the negative CED for  $A = 70$  and the large, positive CED for  $A = 74$  are correctly obtained.

We now analyze the results by looking at the components. Figure 3 shows the total CED denoted by  $V_{CM+ls+ll}$ , and the separated multipole, spin-orbit, and orbital parts by  $V_{CM}$ ,  $\epsilon_{ls}$ , and  $\epsilon_{ll}$ , respectively. For the  $A = 66$  pair  $^{66}\text{As}/^{66}\text{Ge}$ , the spin-orbit component  $\epsilon_{ls}$  has a negative value for the  $J = 0, 2$  and  $4$  states, while the other two,  $V_{CM}$  and  $\epsilon_{ll}$ , are positive. Since the positive values cancel out the negative ones, the net CED are small and positive. At  $J = 6$ , the sudden change from this behavior can be understood as the fact that the involving states are not the first, but the second  $6^+$  states in the  $A = 66$  pair. The values for the  $A = 70$  pair  $^{70}\text{Br}/^{70}\text{Se}$  are large and negative for  $\epsilon_{ls}$ , but positive for  $V_{CM}$  and nearly zero for  $\epsilon_{ll}$ . Since the absolute values of  $\epsilon_{ls}$  are larger, the total CED are therefore negative. This suggests that the spin-orbit contribution is responsible for the observed negative CED in  $^{70}\text{Br}/^{70}\text{Se}$ . For the  $A = 74$  pair  $^{74}\text{Rb}/^{74}\text{Kr}$ , the components indicate a similar overall behavior as those of the lower spin states in the  $A = 66$  pair. However, both  $V_{CM}$  and  $\epsilon_{ll}$  are found larger in the  $A = 74$  pair, and thus are dominant in the summation. Therefore, the  $A = 74$  CED are large and positive. For  $^{78}\text{Y}/^{78}\text{Sr}$ , all components are small, and the total CED therefore indicate small and positive values.

Our calculation suggests that for all the pairs studied, the spin-orbit component,  $\epsilon_{ls}$ , is negative. The effect is particularly enhanced for  $A = 70$ . Thus the spin-orbit term appears to be the origin of the observed CED anomaly in  $^{70}\text{Br}/^{70}\text{Se}$ . But why the absolute values of the spin-orbit component are anomalously large only for  $^{70}\text{Br}/^{70}\text{Se}$ ? We previously mentioned that the spin-orbit term affects single-particle corrections differently for neutrons and protons. We may discuss these with the following estimate. Due to this interaction, the proton  $g_{9/2}$  orbit is lowered by about 66 keV, while the  $f_{5/2}$  orbit is raised by about 66 keV. Then the energy gap between the proton  $g_{9/2}$  and  $f_{5/2}$  orbit decreases roughly by 132 keV. On the contrary, the neutron  $g_{9/2}$  orbit is raised by about 55 keV and the  $f_{5/2}$  orbit is lowered by about 55 keV, and therefore,

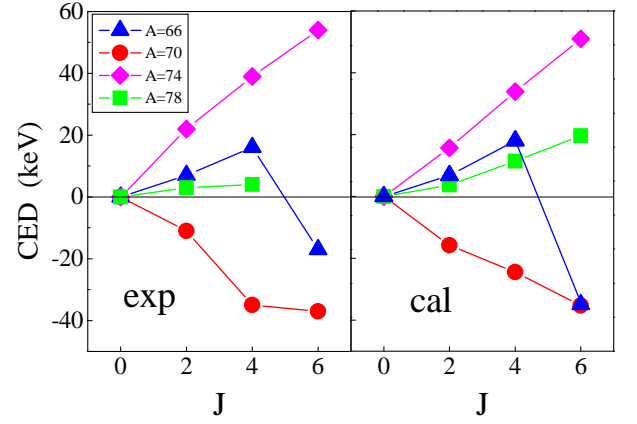


FIG. 2: (Color online) Comparison of calculated CED with experimental data for mass number  $A = 66, 70, 74$ , and  $78$ . Note that for  $A = 66$ , the calculated CED correspond to the second  $6^+$  states.

the spin-orbit contribution enhances the neutron shell gap between the  $g_{9/2}$  and  $f_{5/2}$  orbit roughly by 110 keV. The total effect thus amplifies the difference between the neutron and proton orbits by about 242 keV.

By introducing the difference in neutron occupation number between the ground state of  $0_1^+$  and the excited state with spin  $J$

$$\Delta n_{g_{9/2}}^J = n_{g_{9/2}}^J - n_{g_{9/2}}^{J=0}, \quad (6)$$

it is straightforward to see that the excited states in  $^{70}\text{Se}$  lie higher than those in  $^{70}\text{Br}$  with the same spin, and therefore, CED in Eq. (1) become negative. Since the energy gap between the  $g_{9/2}$  and  $fp$  shell for neutrons is by 242 keV larger than that for protons, the spin-orbit components can be estimated to be -33.4, -58.8, and -77.2 keV for spin  $J = 2, 4$ , and

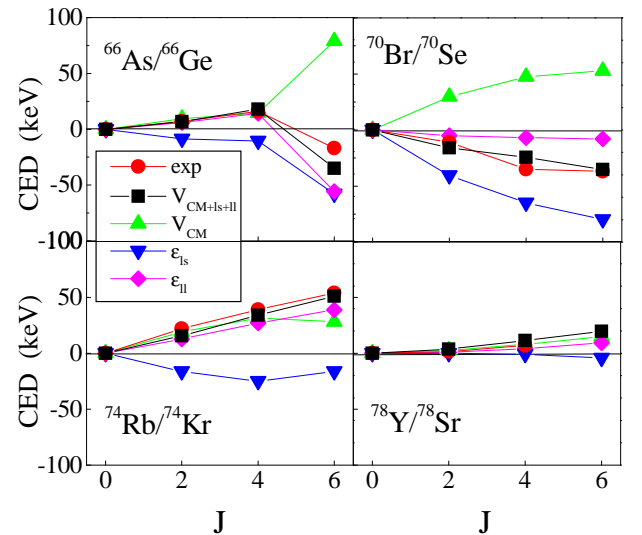


FIG. 3: (Color online) Decomposition of theoretical CED for states shown in Fig. 2 into three terms (see text for explanation). The total CED are denoted by black square symbols.

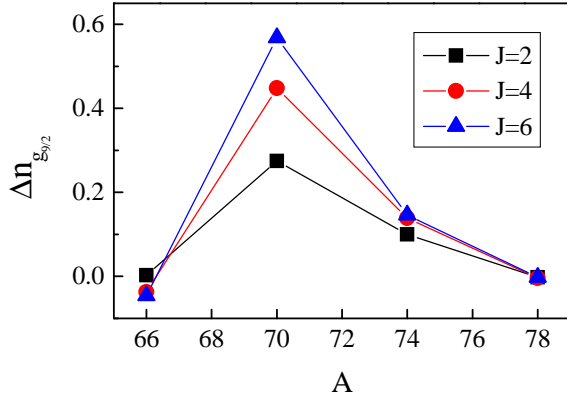


FIG. 4: (Color online) Difference in the neutron occupation number  $n_{g_{9/2}}^J$  between the ground state and the excited states (defined in Eq. (6)) with spin  $J = 2, 4$ , and  $6$  for  $^{66}\text{Ge}$ ,  $^{70}\text{Se}$ ,  $^{74}\text{Rb}$ , and  $^{78}\text{Y}$ .

6 from  $(\Delta n_{g_{9/2}}^J(^{70}\text{Br}) - \Delta n_{g_{9/2}}^J(^{70}\text{Se})) \times 242 \text{ keV}$ , respectively. These values agree well with the calculated spin-orbit components for  $^{70}\text{Br}/^{70}\text{Se}$  in Fig. 3.

Figure 4 shows the differences in neutron occupation number,  $\Delta n_{g_{9/2}}^J$ , between the ground  $0_1^+$  state and the excited  $J$ -states for  $A = 62, 66, 70$ , and  $74$ . One can see that the numbers are larger for  $A = 70$ . The enhanced neutron excitations from the  $fp$  orbits into the  $g_{9/2}$  orbit combined with the single-particle energy shifts  $\epsilon_{ls}$  due to the spin-orbit interaction are the major factors to explain the large negative CED in  $^{70}\text{Br}/^{70}\text{Se}$ . At the mass number  $A = 70$ , the increase of the  $g_{9/2}$  occupation reflects the enhanced excitations from the  $fp$  shell into the  $g_{9/2}$  orbit, which means that  $^{70}\text{Br}$  and  $^{70}\text{Se}$  are transitional nuclei. In fact, it has been known that the  $N = Z$  nuclei around  $A = 70$  such as  $^{68}\text{Se}$  and  $^{72}\text{Kr}$  do not correspond to a single well-developed shape, and may exhibit the phenomenon of oblate-prolate shape coexistence [8–11]. In addition, a shape phase transition with an abrupt change in structure when the proton and neutron numbers cross  $N = Z = 35$  has been suggested [7].

For  $^{70}\text{Se}$ , our calculation with the standard effective charges  $1.5e$  for protons and  $0.5e$  for neutrons obtains  $B(E2, I \rightarrow I-2)$  values of  $345, 539$ , and  $594 e^2 fm^4$  for  $E2$  transitions de-exciting the  $J^\pi = 2_1^+, 4_1^+$ , and  $6_1^+$  states, respectively. These are in a good agreement with the experimental values  $342$  (19),  $370$  (24), and  $530$  (96)  $e^2 fm^4$  found in Ref. [15]. Our calculated spectroscopic quadrupole moments are  $37.5, 50.2$ , and  $55.5 e fm^2$ , respectively for the  $J^\pi = 2_1^+, 4_1^+$ , and  $6_1^+$  states. Using these values and assuming an axial deformation, we may estimate the quadrupole deformation as  $-0.21, -0.22$ , and  $-0.22$  for the  $J^\pi = 2_1^+, 4_1^+$ , and  $6_1^+$  states, respectively, suggesting that the  $^{70}\text{Se}$  yrast states are oblatelly deformed. This is in consistence with the conclusions from the recent measurement [15]. The deformation is roughly constant, and does not show changes with increasing spin. Thus from our shell-model calculation, the negative CED for  $A = 70$  are not attributed to subtle differences in the Coulomb energy as

shapes evolve with spin [5].

In conclusion, by performing modern shell-model calculations, we have investigated the CED effects between the isospin  $T = 1$  states in odd-odd  $N = Z$  nuclei and the isobaric analogue states in their even-even neighbors for the upper  $fp$ -shell nuclei. In order to obtain the  $T = 1$  states for odd-odd  $N = Z$  nuclei, we have gone beyond the usual Lanczos method by employing the filter diagonalization method for the first time in application. It has been shown that the anomalous CED found for the pair  $^{70}\text{Br}$  and  $^{70}\text{Se}$  originates from neutron excitations from the  $fp$ -shell to the  $g_{9/2}$  intruder orbit reflected in a sudden enhancement in the electromagnetic spin-orbit term for  $A = 70$ . The study has shown how the structure changes manifest themselves in a measure of the isospin-symmetry breaking in effective nuclear interactions.

This work was partially supported by the National Natural Science Foundation of China under contract No. 11075103 and 11135005.

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